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SIMULATION OF A MATHEMATICAL MODEL FOR SOIL BIOREMEDIATION

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Abstract. The article presents some simulations for a mathematical model that describes the bioremediation of a polluted soil. The mathematical model is a reaction-diffusion system for the pollutant and for the bacteria. We made some two-dimensional simulations that show us how a small parameter affects the coupling and diffusion. The simulations help us to visualize both pollutant and bacteria evolution.

1. **Introduction**

The objective of this article is to study a mathematical model that describes the bioremediation of agricultural or urban soils, an environment that is contaminated with heavy metals and has recognized toxic potential. Metals are natural components that are part of global ecosystems. In principle, among the 53 known heavy metals, some are essential for the proper development of living organisms, but in rather small concentrations [1]. However, most can be toxic, even at extremely low concentrations, the impact they have on human and animal health being aggravated by their long-term resistance in the environment.

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Two of the most present heavy metals in the soil are cadmium (Cd) and chromium (Cr), which can reach the soil as a result of industrial emissions, industrial waste, the use of fertilizers, pesticides or other anthropogenic activities [9]; [1].

The presence of cadmium and chromium both in soil and in the human organism is strictly regulated by international standards developed by WHO (2002) and USEPA (2002), their presence being closely correlated with the detection of carcinogenic diseases in humans.

After entering the soil, pollutants can undergo transport, transformation, transfer or accumulation and fixation phenomena. All these phenomena contribute to their spread and distribution in the soil elements, to the modification of the chemical structure of the soil. The transport of pollutants consists of the movement of pollutants in the soil, relative to the source. The movement of pollutants is achieved through the phenomena of [2]; [4]:

- diffusion - the movement of pollutant molecules in the direction of decreasing concentration, favored by the concentration gradient (which determines Fick-type diffusion), temperature or pressure;
- convection - the horizontal movement of the pollutant together with the carrier fluid, air or water, in the direction of fluid movement.

Given the negative impact of heavy metals (pollutants) on human health, a particularly important concern is to find methods to remove pollutants from the environment in which they act (water, soil) by applying techniques that involve minimal costs and without further polluting the environment. In addition to classic pollution remediation technologies, such as extraction, separation, destruction, immobilization, innovative technologies for bioremediation of polluted environments are being increasingly used [3]. Bioremediation of a polluted environment consists of using the natural biological activity of plants and microorganisms to destroy the pollutant. Given that microorganisms can be isolated under almost any environmental condition, the aim is to introduce nutrients and oxygen into the contaminated environment, in order to create favorable conditions for life and the bioremediation process [10], [7]. Sometimes, to increase the effectiveness of bioremediation, microorganisms adapted to degrade certain pollutants are used.

Microorganisms move in the environment polluted by heavy metals either by diffusion or by chemotaxis. Chemotaxis represents the biological phenomenon of changing the direction of the population of microorganisms (bacteria) in response to the influence of a pollutant in the given environment. The increase in the concentration gradient of the pollutant leads to the polarization of the movement of microorganisms and allows their accumulation in areas with an increased concentration of the pollutant.

From a mathematical point of view, bioremediation processes with the help of microorganisms moving by diffusion and chemotaxis are represented by systems of partial derivatives written for the concentrations of the pollutant and microorganisms, together with initial and boundary conditions. The first mathematical models for chemotaxis are found in the works of Patlak [8] and Keller and Segel [5]; [6].

2. **Mathematical model**

Let us consider the mathematical model of an isotropic, nondeformable and homogeneous porous soil in which a single type of pollutant (heavy metal) acts. We assume that in this environment a bacteria acts and is capable of neutralizing the pollutant.

Let us consider a pollutant that acts in a domain denoted by Ω open and bounded in $\mathbb{R}$ that has a sufficiently smooth boundary $\Gamma = \partial\Omega$ (of class C^1). The geometry of Ω with the boundary Γ is supposed to be known. We denote by t the time variable that runs within the interval $(0,T)$ with T finite, and by ξ the spatial coordinate. Thus we denote by $p\,(t,\xi)$ and by $b\,(t,\xi)$ the concentration of the pollutant and of the bacteria. The diffusion coefficients for the pollutant and for the bacteria, denoted by $\delta > 0$, $D > 0$, are supposed to be constants and the chemotactic response is denoted by the function $K\,(b,p)$.

The mathematical model of infiltration for the pollutant is described by the a system with homogeneous Dirichlet boundary conditions:

$$\begin{aligned} \frac{\partial p}{\partial t} - \delta\Delta p &= \phi\,(b,p)\,, \quad (t,\xi) \in (0,T)\times\Omega, \\ p\,(0,\xi) &= p_0\,(\xi) \text{ in } \Omega, \\ p\,(t,\xi) &= 0 \text{ on } \Gamma. \end{aligned} \tag{1}$$

The model for bacteria that is moving by diffusion and chemotaxis is given by the next system with homogeneous Dirichlet boundary conditions:

$$\begin{aligned} \frac{\partial b}{\partial t} - D\Delta b + \nabla\cdot[bK(b,p)\nabla p] &= f\,(b,p)\,, \quad (t,\xi) \in (0,T)\times\Omega, \\ b\,(0,\xi) &= b_0\,(\xi) \text{ in } \Omega, \\ p\,(t,\xi) &= 0 \text{ on } \Gamma. \end{aligned} \tag{2}$$

Thus, the model to be studied is a nonlinear problem with initial conditions.

3. **The dimensionless mathematical model**

In order to give some results about the systems using the small parameters method we write the dimensionless form. Let be L_c, T_c, P_c, B_c, D_c, δ_c, K_c, Φ_c, F_c the characteristic scale for length, time, pollutant and bacteria concentration, diffusion coefficients, chemotactic response and for the functions that describe the multiplication and destruction of the pollutant and bacteria.

We define the dimensionless variables $\widetilde{\xi} = \frac{\xi}{L_c}$, $\widetilde{t} = \frac{t}{T_c}$, $\widetilde{p} = \frac{p}{P_c}$, $\widetilde{b} = \frac{b}{B_c}$, $\widetilde{D} = \frac{D}{D_c}$, $\widetilde{\delta} = \frac{\delta}{\delta_c}$, $\widetilde{K} = \frac{K}{K_c}$, $\widetilde{\varphi} = \frac{\varphi}{\Phi_c}$, $\widetilde{f} = \frac{f}{F_c}$. Computing all the derivatives in term of the new variables we substitute in the equations. First, for the pollutant system we get:

$$\frac{P_c}{T_c}\frac{\partial\widetilde{p}}{\partial\widetilde{t}} - \widetilde{\delta}\delta_c\frac{P_c}{L_c^2}\Delta\widetilde{p} = \Phi_c\widetilde{\varphi}\left(\widetilde{b}B_c, \widetilde{p}P_c\right),$$

and multiplying by $\frac{T_c}{P_c}$ we obtain:

$$\frac{\partial\widetilde{p}}{\partial\widetilde{t}} - \frac{\delta_c T_c}{L_c^2}\widetilde{\delta}\Delta\widetilde{p} = \frac{\Phi_c T_c}{P_c}\widetilde{\varphi}^*\left(\widetilde{b}, \widetilde{p}\right).$$

In the equation above we denote $\overline{\delta} := \frac{\delta_c T_c}{L_c^2}$ and $\overline{\varphi} := \frac{\Phi_c T_c}{P_c}$. The initial and the limit conditions become:

$$\widetilde{p}\left(0,\xi\right) = \widetilde{p}_0\left(\xi\right) \text{ for } \widetilde{\xi} \in \widetilde{\Omega} \text{ and } \widetilde{p}\left(t,\xi\right) = 0 \text{ on } \widetilde{\Gamma}.$$

Similarly, for the bacteria equation we get

$$\frac{B_c}{T_c}\frac{\partial\widetilde{b}}{\partial\widetilde{t}} - \widetilde{D}D_c\frac{B_c}{L_c^2}\Delta\widetilde{b} + \frac{K_c P_c}{L^2}\widetilde{\nabla}\cdot\left[\widetilde{K}\left(\widetilde{b}, \widetilde{p}\right)\widetilde{\nabla}\widetilde{p}\right] = F_c\widetilde{f}\left(\widetilde{b}B_c, \widetilde{p}P_c\right),$$

and multiplying by $\frac{T_c}{B_c}$ we obtain:

$$\frac{\partial\widetilde{b}}{\partial\widetilde{t}} - \frac{D_c T_c}{L_c^2}\widetilde{D}\Delta\widetilde{p} + \frac{K_c P_c T_c}{B_c L^2}\widetilde{\nabla}\cdot\left[\widetilde{K}\left(\widetilde{b}, \widetilde{p}\right)\widetilde{\nabla}\widetilde{p}\right] = \frac{F_c T_c}{B_c}\widetilde{f}\left(\widetilde{b}B_c, \widetilde{p}P_c\right).$$

In the last equation we denote by $\overline{D} := \frac{D_c T_c}{L_c^2}$ the diffusion parameter, by $\overline{K} := \frac{K_c P_c T_c}{B_c L^2}$ the chemotaxis parameter and by $\overline{f} := \frac{F_c T_c}{B_c}$. The initial and the limit conditions become:

$$\widetilde{b}\left(0,\xi\right) = \widetilde{b}_0\left(\xi\right) \text{ for } \widetilde{\xi} \in \widetilde{\Omega} \text{ and } \widetilde{b}\left(t,\xi\right) = 0 \text{ on } \widetilde{\Gamma}.$$

Finally, without writing the suprascript ˜ for simplicity we have the next dimenssionless system which has two parts, one for pollutant and one for bacteria:

$$\frac{\partial p}{\partial t} - \overline{\delta}\delta\Delta p = \overline{\varphi}\varphi\left(b,p\right),$$
$$p\left(0,\xi\right) = p_0\left(\xi\right) \text{ for } \xi \in \Omega,$$
$$p\left(t,\xi\right) = 0 \text{ on } \Gamma,$$

and

$$\frac{\partial b}{\partial t} - \overline{D}D\Delta p + \overline{K}\nabla \cdot \left[K\left(b,p\right)\nabla p\right] = \overline{f}f\left(b,p\right),$$
$$b\left(0,\xi\right) = b_0\left(\xi\right) \text{ for } \xi \in \Omega,$$
$$b\left(t,\xi\right) = 0 \text{ on } \Gamma.$$

In this system we can consider the small parameters $\overline{\delta}$, $\overline{\varphi}$, $\overline{D}$, $\overline{K}$, $\overline{f}$. The model with small paratanaers $\overline{\delta}$, $\overline{\varphi} = \varepsilon$ was studied in [11]. In this paper we consider that $\overline{D} = \overline{K} = \overline{f} = \varepsilon$, for ε small. All the other parameters are considered to be of first order.

4. **Description and parameter selection. Simulation study**

In this simulation study we consider a two-component reaction-diffusion system: one partial differential equation given for the pollutant $p(t, \varepsilon)$ and one for the bacteria $b(t, \varepsilon)$, with small parameter ε. Simplifying assumptions for simulation we consider that the pollutant is consumed by bacteria and the bacteria grows by consuming pollutant. In this way we set the functions $\varphi\left(b,p\right) = -bp$ and $f\left(b,p\right) = bp$.

We also consider that $K\left(b,p\right) = 1$ for simplicity and we fix $\delta = 0.1$. The domain is two-dimensional denoted by $\Omega = \left(0,1\right) \times \left(0,1\right)$. The time t runs in the interval $[0; 0.5]$ and we make simulations for bacteria and for pollutant at fixed moments $t = 0;\ 0.1;\ 0.25;\ 0.5$. The method we used is 2D finite difference method.

With this simulation we can explain how the pollutant and bacteria evolve differently as ε increases. To perform the simulations we used FiPy which is a free, open-source Python library specifically designed for PDEs, especially reaction–diffusion systems using numerical methods.

The *Figure 1* represents the simulation for $\varepsilon = 0.01$ on the first line for bacteria and on the second one for the pollutant.

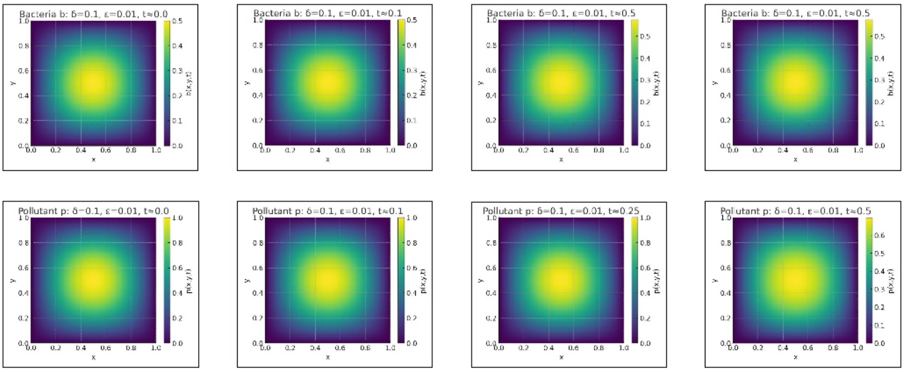


FIGURE 1. Simulation of the bacteria and the pollutant for $\varepsilon = 0.01$

As we can observe the pollutant and the bacteria have a very small interaction. This means that the pollutant diffuses slowly and is only slightly consumed by the bacteria. The bacteria growth is also minimal, staying close to the initial distribution. Overall, the system remains close to the initial conditions over the $t = 0.5s$ time frame.

Figure 2 represents the simulation for $\varepsilon = 0.05$.

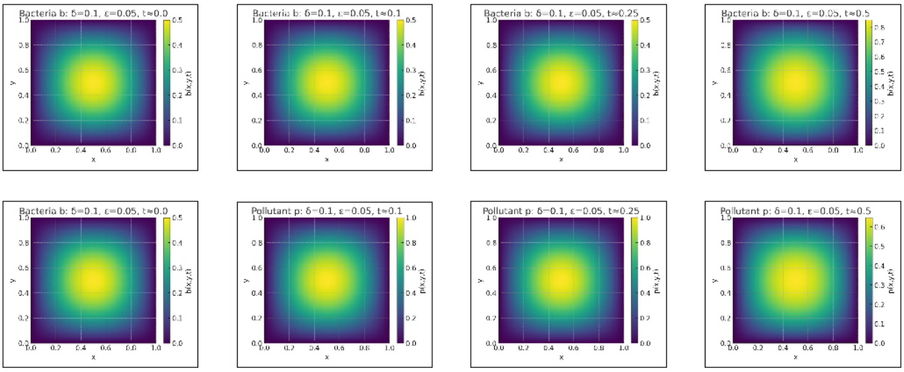
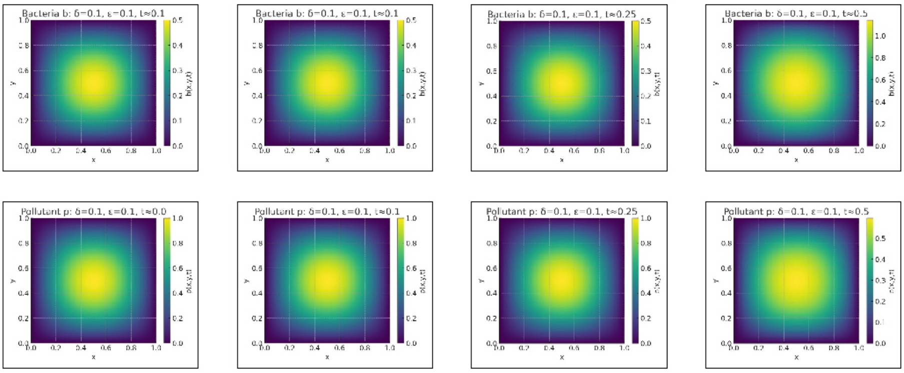


FIGURE 2. Simulation of the bacteria and the pollutant for $\varepsilon = 0.05$

In this case we have a moderate interaction. That means that the pollutant p starts to decrease faster, especially near the center of the domain where the initial concentration is highest. Bacteria b grows more noticeably, forming a clear concentration peak around the center region. There's a visible spatial interaction between bacteria and pollutant as bacteria grow, they locally deplete the pollutant.

The *Figure 3* represents the simulation for $\varepsilon = 0.1$.



Bacteria b: δ=0.1, ε=0.1, t≈0.1

Bacteria b: δ=0.1, ε=0.1, t≈0.1

Bacteria b: δ=0.1, ε=0.1, t≈0.25

Bacteria b: δ=0.1, ε=0.1, t≈0.5

Pollutant p: δ=0.1, ε=0.1, t≈0.0

Pollutant p: δ=0.1, ε=0.1, t≈0.1

Pollutant p: δ=0.1, ε=0.1, t≈0.25

Pollutant p: δ=0.1, ε=0.1, t≈0.5

Figure 3. Simulation of the bacteria and the pollutant for $\varepsilon = 0.1$

In this case we can observe a stronger interaction. The concentration p of the pollutant decays much faster, significantly reduced at the moment $t = 0.25$ and almost depleted at the moment $t = 0.5$. The concentration b of the bacterial population grows rapidly, reaching higher concentrations and forming sharper peaks. In this case the system shows strong nonlinear coupling, with bacteria dynamics strongly driven by the rapid pollutant consumption.

5. **Conclusions**

The simulations help us to visualize both pollutant and bacteria evolution, showing how the small parameter ε affects the coupling and diffusion. As ε increases, the rate of interaction between pollutant and bacteria accelerates, leading to faster pollutant depletion and faster bacterial proliferation.

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